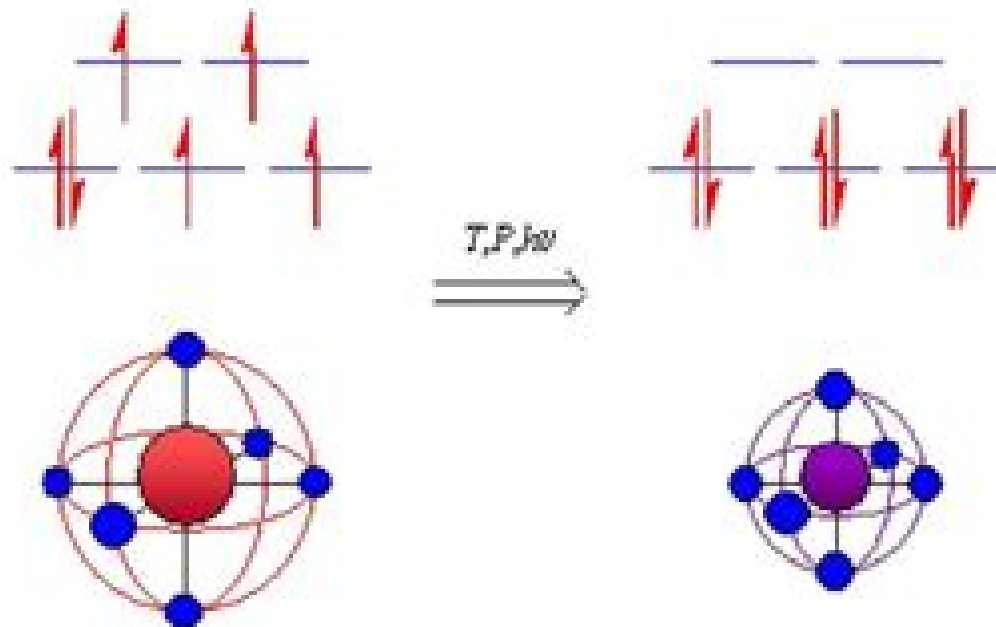


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Marcel Swart, Miquel Costas



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Spin States in Biochemistry and Inorganic Chemistry Marcel Swart, Miquel Costas, 2015-09-17 It has long been recognized that metal spin states play a central role in the reactivity of important biomolecules in industrial catalysis and in spin crossover compounds As the fields of inorganic chemistry and catalysis move towards the use of cheap non toxic first row transition metals it is essential to understand the important role of spin states in influencing molecular structure bonding and reactivity Spin States in Biochemistry and Inorganic Chemistry provides a complete picture on the importance of spin states for reactivity in biochemistry and inorganic chemistry presenting both theoretical and experimental perspectives The successes and pitfalls of theoretical methods such as DFT ligand field theory and coupled cluster theory are discussed and these methods are applied in studies throughout the book Important spectroscopic techniques to determine spin states in transition metal complexes and proteins are explained and the use of NMR for the analysis of spin densities is described Topics covered include DFT and ab initio wavefunction approaches to spin states Experimental techniques for determining spin states Molecular discovery in spin crossover Multiple spin state scenarios in organometallic reactivity and gas phase reactions Transition metal complexes involving redox non innocent ligands Polynuclear iron sulfur clusters Molecular magnetism NMR analysis of spin densities This book is a valuable reference for researchers working in bioinorganic and inorganic chemistry computational chemistry organometallic chemistry catalysis spin crossover materials materials science biophysics and pharmaceutical chemistry

Fundamentals of Porphyrin Chemistry Penelope J. Brothers, Mathias O. Senge, 2022-06-21 FUNDAMENTALS OF PORPHYRIN CHEMISTRY An indispensable and concise overview of the chemistry of porphyrins and related molecules In Fundamentals of Porphyrin Chemistry A 21st Century Approach a team of distinguished researchers delivers a compact and accessible introduction to the broad field of porphyrin chemistry It discusses the basics of porphyrin synthesis and structure as well as that of related molecules and the current and future roles that porphyrins play in chemical transformations materials design and synthesis energy capture and transduction human health and the environment This edited volume is a self contained tutorial on concepts of critical importance to porphyrin chemistry and serves as the foundation for discussions about the applications of porphyrin related compounds found in the second volume This book contains A thorough introduction to porphyrins including their structure nomenclature naturally occurring porphyrins synthetic porphyrins and common families of porphyrin related compounds Comprehensive explorations of chemical porphyrin synthesis including how to synthesize porphyrins from simple symmetric and advanced ABCD substituted porphyrins Practical discussions of the physical characteristics of porphyrins including their structural features electronic structure spectroscopy magnetism electrochemistry and electron transfer processes Perfect for experienced academic researchers in the field of porphyrin chemistry seeking a quick reference Fundamentals of Porphyrin Chemistry A 21st Century Approach is also an indispensable resource for researchers new to the field who need an overview

directing them to literature in more focused areas *NMR Spectroscopy Explained* Neil E. Jacobsen, 2007-08-27 NMR Spectroscopy Explained Simplified Theory Applications and Examples for Organic Chemistry and Structural Biology provides a fresh practical guide to NMR for both students and practitioners in a clearly written and non mathematical format It gives the reader an intermediate level theoretical basis for understanding laboratory applications developing concepts gradually within the context of examples and useful experiments Introduces students to modern NMR as applied to analysis of organic compounds Presents material in a clear conversational style that is appealing to students Contains comprehensive coverage of how NMR experiments actually work Combines basic ideas with practical implementation of the spectrometer Provides an intermediate level theoretical basis for understanding laboratory experiments Develops concepts gradually within the context of examples and useful experiments Introduces the product operator formalism after introducing the simpler but limited vector model *Computational Chemistry*, 2019-02-20 Computational Chemistry Volume 73 the latest release in the Advances in Inorganic Chemistry series presents timely and informative summaries on current progress in a variety of subject areas This acclaimed serial features reviews written by experts in the field serving as an indispensable reference to advanced researchers that empowers readers to pursue new developments in each field Users will find this to be a comprehensive overview of recent findings and trends from the last decade that covers various kinds of inorganic topics from theoretical oriented supramolecular chemistry to the quest for accurate calculations of spin states in transition metals Features comprehensive reviews on the latest developments in computational studies in inorganic chemistry Includes contributions from leading experts in the field of inorganic reaction mechanisms Serves as an indispensable reference to advanced researchers in many related fields Essentials of Chemical Biology Andrew D. Miller, Julian A. Tanner, 2024-01-31 Essentials of Chemical Biology Discover a detailed knowledge of concepts and techniques that shape this unique multi discipline Chemical Biology is devoted to understanding the way that Biology works at the molecular level This is a problem driven multi discipline incorporating as it does Organic Physical Inorganic and Analytical Chemistry alongside newer emerging molecular disciplines In recent years Chemical Biology has emerged as a vibrant and growing multi discipline distinct from Biochemistry that is focused on the quantitative analyses of the structures and functions of biological macromolecules and macromolecular lipid assemblies at first in isolation then in vitro and in vivo The second edition of the Essentials of Chemical Biology begins with a thorough introduction to the structure of biological macromolecules and macromolecular lipid assemblies before moving on to the principles of chemical and biological synthesis followed by descriptions of a comprehensive variety of research techniques and experimental methods In addition the second edition now includes new sections on the behaviour of biological macromolecules and macromolecular lipid assemblies in cells in vitro and in organisms in vivo Given this the second edition of the Essentials of Chemical Biology promises to cement itself as the leading introduction to Chemical Biology incorporating descriptions of cutting edge research wherever appropriate Hence

readers of the second edition of the Essentials of Chemical Biology will find a general expansion in understanding of basic molecular mechanisms in Biology moving towards cellular and organismal mechanisms entirely new chapters covering miniaturization and array technologies Chemical Cell Biology and the interface between Chemical Biology and Nanotechnology updates to chapters reflecting recent research developments an increased engagement with medical applications Essentials of Chemical Biology is ideal for advanced undergraduates or post graduate students in Chemical Biology and adjacent fields

Molybdenum and Tungsten Enzymes Russ Hille, Carola Schulzke, Martin L Kirk, 2016-10-10

There has been enormous progress in our understanding of molybdenum and tungsten enzymes and relevant inorganic complexes of molybdenum and tungsten over the past twenty years This set of three books provides a timely and comprehensive overview of the field and documents the latest research Building on the first and second volumes that focussed on biochemistry and bioinorganic chemistry aspects the third volume focusses on spectroscopic and computational methods that have been applied to both enzymes and model compounds A particular emphasis is placed on how these important studies have been used to reveal critical components of enzyme mechanisms This text will be a valuable reference to workers both inside and outside the field including graduate students and young investigators interested in developing new research programs in this area

Scanning Transmission Electron Microscopy Stephen J. Pennycook, Peter D. Nellist, 2011-03-24

Scanning transmission electron microscopy has become a mainstream technique for imaging and analysis at atomic resolution and sensitivity and the authors of this book are widely credited with bringing the field to its present popularity Scanning Transmission Electron Microscopy STEM Imaging and Analysis will provide a comprehensive explanation of the theory and practice of STEM from introductory to advanced levels covering the instrument image formation and scattering theory and definition and measurement of resolution for both imaging and analysis The authors will present examples of the use of combined imaging and spectroscopy for solving materials problems in a variety of fields including condensed matter physics materials science catalysis biology and nanoscience Therefore this will be a comprehensive reference for those working in applied fields wishing to use the technique for graduate students learning microscopy for the first time and for specialists in other fields of microscopy

Introduction to Functional Magnetic Resonance Imaging Richard B. Buxton, 2009-08-27

Functional Magnetic Resonance Imaging fMRI has become a standard tool for mapping the working brain s activation patterns both in health and in disease It is an interdisciplinary field and crosses the borders of neuroscience psychology psychiatry radiology mathematics physics and engineering Developments in techniques procedures and our understanding of this field are expanding rapidly In this second edition of Introduction to Functional Magnetic Resonance Imaging Richard Buxton a leading authority on fMRI provides an invaluable guide to how fMRI works from introducing the basic ideas and principles to the underlying physics and physiology He covers the relationship between fMRI and other imaging techniques and includes a guide to the statistical analysis of fMRI data This

book will be useful both to the experienced radiographer and the clinician or researcher with no previous knowledge of the technology **Advances in Imaging and Electron Physics** ,2013-01-17 Advances in Imaging and Electron Physics features cutting edge articles on the physics of electron devices especially semiconductor devices particle optics at high and low energies microlithography image science and digital image processing electromagnetic wave propagation electron microscopy and the computing methods used in all these domains Contributions from leading authorities Informs and updates on all the latest developments in the field Chemical Generation and Reception of Radio-and Microwaves Anatoly L. Buchachenko,Eugene L. Frankevich,1996-12-17 Mit diesem ersten kritischen berblick seit ber einem Jahrzehnt leisten zwei international anerkannte Autorit ten auf dem Feld der Spin Physik einen wichtigen Beitrag zu diesem aktuellen Feld der Chemischen Physik Sie bechreiben zwei berraschende Charakteristika chemischer Reaktionen Die Erzeugung von Radiowellen und umgekehrt der Einflu von elektromagnetischen Wellen auf chemische Reaktionen In diesem Sinne etabliert dieses Werk die chemische Radiophysik als ein neues Gebiet der Chemischen Physik Die Autoren schildern detailliert die Mechanismen von chemischen und physikalischen Reaktionen die Auswahl von Kernen durch Spinorientierung und magnetische Momente die nicht magnetische Trennung von Isotopen und deren Akkumulation in den Reaktionsprodukten Damit werden neue Einsichten in die chemische Dynamik und Reaktionsmechanismen vermittelt Die chemische Radiophysik bietet neue radiospektroskopische Verfahren mit hoher Empfindlichkeit Ein kurzes Kapitel fa t die physikalischen Grundlagen zusammen aufgrund derer elektromagnetische Felder biologisch relevante Reaktionen hervorrufen k nnen Chemical Generation and Reception of Radio and Microwaves ist eine wichtige Referenz f r Chemische Physiker f r Physikalische Organische Chemiker Materialwissenschaftler sowie Radio und Biophysiker

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